Supplementary Information for:

An Efficient Chiral Moderator Prepared from Inexpensive (+)-3-Carene: Synthesis of the HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitor DPC 963

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X-ray Crystal Structure Analysis for Compound 7

CRYSTAL DATA: $C_{14}H_{25}O_2N_1$ from ^{i}ProAc/heptanes , colorless , rod , ~0.08 x 0.12 x 0.55 mm, monoclinic , P21 (No. 4), a = 13.987(4)Å, b = 6.127(1)Å, c = 32.581(9)Å, beta = 97.69(1)°, T = -100°C, Vol = 2767.0Å^3, Z = 8, Formula weight = 239.36, Density = 1.149 g/cc, μ(Mo) = 0.71 cm^{-1}

DATA COLLECTION: Rigaku RU300, R-AXIS image plate area detector, MoKalpha radiation ,filament size = 12.0 x 2.0mm, anode power = 55kV x 240mA, crystal to plate distance = 85.0mm, 105μ pixel raster, number of frames = 45, oscillation range = 4.0%deg;, exposure time = 25.0 min/frame, box sum integration, data collected = 10173, 2-theta range = 3.0° - 48.2°, maximum hkl = 15 6 37, no absorption correction, 3729 duplicates, 2.5% R-merge, 4985 unique reflections with I> 2.5sig(I),

SOLUTION AND REFINEMENT: Structure solved by direct methods using teXsan(SIR-92), refined using Z program suite(Calabrese), refinement by full-matrix least squares on F, scattering factors from Int. Tables for X-ray Crystallography, Vol IV, biweight ~ [sigma 2(I)+0.0009I 2]-1/2, refined 68 of 168 atoms, 68 atoms refined anisotropic, 612 parameters, data/parameter ratio = 8.11, final R1 = 0.042, Rw = 0.037, error of fit = 1.41, max shift/error = 0.01, largest residual density = 0.19e/Å3, near H9'. Because the refinement for a few of the hydrogen atoms gave unrealistic C-H bond distances (1.11A), all of the hydrogens have been idealized close to their previously refined positions.

RESULTS: The asymmetric unit contains four molecules as shown in figure 1 with thermal ellipsoids drawn to the 50% probability level. The four molecules form an infinite pseudo 31 screw arrangement along the b-axis. The hydrogen bonded infinite chain explains why the crystals form as b-axis needles and were difficult to grow. The enantiomeric setting was previously known and set for this refinement. The conformation of the first three molecules of the asymmetric unit have similar environments around the pseudo 31 axis and form nice chair conformations for the caranol ring (C1-C2- C3-C4-C7-C5-C6). The fourth molecule is slightly different and has the O-H/methyl groups tilted, distorting the chair conformation and putting the O-H group in a pseudo equatorial arrangement. To ensure that the structure was in the correct space group (not trigonal), the environment around the morpholino oxygen atoms was carefully examined. Only O14 is in a hydrogen bond acceptor environment. Therefore the 31 screw is not a crystallographic 31 screw.

TABLE I. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

ATOM	X	Y	Z	BISO
O(2)	2971(2)	1081(0)	1842(1)	2.0(1)’
O(14)	416(2)	1141(5)	3153(1)	3.7(1)’
O(22)	4227(2)	-2360(4)	2168(1)	2.2(1)’
O(34)	8535(2)	-2948(5)	2505(1)	3.5(1)’
O(42)	4172(2)	4360(4)	1552(0)	2.1(1)’
O(54)	2359(2)	3875(5)	-201(1)	3.0(1)’
O(62)	8873(2)	-292(5)	3692(1)	3.2(1)’
O(74)	11611(2)	5252(6)	4305(1)	4.8(1)’
N(11)	1225(2)	1003(5)	2392(1)	2.0(1)’
N(31)	6498(2)	-2803(5)	2540(1)	1.9(1)’
N(51)	3620(2)	3999(5)	564(1)	1.7(1)’
N(71)	9841(2)	2947(5)	4221(1)	2.5(1)’
C(1)	1348(2)	428(5)	1958(1)	1.7(1)’
C(2)	2016(2)	2018(5)	1765(1)	1.8(1)’
C(2’)	2055(2)	4319(6)	1949(1)	2.2(1)’
C(3)	1733(2)	2185(6)	1290(1)	1.9(1)’
C(4)	1458(3)	27(6)	1091(1)	2.1(1)’
C(5)	668(2)	-1127(6)	1287(1)	2.1(1)’
C(6)	402(2)	-4(6)	1669(1)	2.1(1)’
C(7)	469(2)	-299(6)	846(1)	2.1(1)’
C(8)	413(3)	-2074(7)	518(1)	3.5(1)’
C(9)	-190(3)	1578(6)	720(1)	2.7(1)’
C(12)	388(3)	2367(6)	2443(1)	2.4(1)’
C(13)	429(3)	3022(6)	2892(1)	3.3(1)’
C(15)	1203(3)	-266(7)	3097(1)	3.4(1)’
C(16)	1177(3)	-953(6)	2650(1)	2.4(1)’
C(21)	5562(2)	-3209(6)	2684(1)	2.0(1)’
C(22)	4784(3)	-1434(6)	2542(1)	2.1(1)’
C(22’)	5188(3)	733(6)	2429(1)	3.0(1)’
C(23)	4090(3)	-1084(6)	2860(1)	2.5(1)’
C(24)	3795(3)	-3181(6)	3050(1)	2.6(1)’
C(25)	4640(3)	-4589(6)	3224(1)	2.4(1)’
C(26)	5604(3)	-3708(6)	3150(1)	2.3(1)’
C(27)	3990(3)	-3620(7)	3513(1)	3.1(1)’
C(28)	4342(3)	-1829(7)	3814(1)	4.2(1)’
C(29)	3315(3)	-5210(8)	3679(1)	4.6(1)’
C(32)	7000(3)	-4810(6)	2445(1)	2.3(1)’
C(33)	7868(3)	-4266(6)	2245(1)	2.8(1)’
C(35)	8072(3)	-1030(6)	2619(1)	3.0(1)’
C(36)	7193(3)	-1521(6)	2823(1)	2.2(1)’
C(41)	4496(2)	3597(5)	863(1)	1.6(1)’
C(42)	4655(2)	5288(5)	1224(1)	1.7(1)’
C(42’)	4217(3)	7516(6)	1115(1)	2.3(1)’
C(43)	5723(2)	5523(6)	1383(1)	1.9(1)’
C(44)	6263(2)	3399(6)	1407(1)	1.9(1)’
C(45)	6138(3)	2134(6)	1002(1)	2.1(1)’
C(46)	5424(2)	3201(6)	675(1)	2.1(1)’
C(47)	7114(2)	2994(6)	1176(1)	2.1(1)’
C(48)	7799(3)	1243(6)	1362(1)	2.9(1)’
C(49)	7596(3)	4827(6)	979(1)	2.7(1)’
C(52)	3174(3)	1979(6)	399(1)	2.1(1)’
C(53)	2224(3)	2454(6)	137(1)	2.8(1)’

TABLE II. Fractional Coordinates (X10000) and Isotropic Thermal Parameters

C(55)	2812(3)	5833(6)	-47(1)	2.8(1)’
C(56)	3775(3)	5366(5)	208(1)	2.1(1)’
C(61)	8930(3)	1977(6)	4302(1)	2.5(1)’
C(62)	8334(3)	1282(6)	3892(1)	2.5(1)’
C(62’)	8111(3)	3173(6)	3591(1)	3.4(1)’
C(63)	7416(3)	90(7)	3973(1)	3.7(1)’
C(64)	7118(3)	111(6)	4403(1)	3.7(1)’
C(65)	7558(3)	1776(7)	4715(1)	3.5(1)’
C(66)	8313(3)	3249(6)	4576(1)	3.1(1)’
C(67)	6509(3)	1892(7)	4568(1)	4.0(1)’
C(68)	6103(3)	3681(8)	4287(1)	5.3(2)’
C(69)	5851(4)	1137(8)	4877(1)	5.8(2)’
C(72)	10672(3)	2177(7)	4499(1)	3.7(1)’
C(73)	11586(3)	2960(9)	4343(1)	4.9(2)’
C(75)	10773(3)	5985(7)	4050(1)	4.0(1)’
C(76)	9885(3)	5314(7)	4210(1)	3.4(1)’

TABLE III. Anisotropic Thermal Parameters (Å² X 1000)
exp[-19.739(U11hha*a*...+2(U12hka*b*...))]

ATOM	U11	U22	U33	U12	U13	U23
O(2)	18(2)	28(1)	32(1)	0(1)	4(1)	5(1)
O(14)	68(2)	48(2)	27(1)	-3(2)	20(1)	0(1)
O(22)	31(2)	24(1)	26(1)	1(1)	-7(1)	-4(1)
O(34)	35(2)	54(2)	44(1)	-5(1)	5(1)	-13(1)
O(42)	37(2)	25(1)	19(1)	-3(1)	9(1)	0(1)
O(54)	42(2)	42(1)	26(1)	-1(1)	-5(1)	5(1)
O(62)	55(2)	36(1)	34(1)	2(1)	10(1)	-6(1)
O(74)	58(3)	73(2)	51(2)	-28(2)	13(1)	-14(1)
N(11)	29(2)	28(2)	18(1)	0(1)	6(1)	1(1)
N(31)	21(2)	27(1)	23(1)	-2(1)	-1(1)	-2(1)
N(51)	21(2)	22(1)	23(1)	1(1)	3(1)	3(1)
N(71)	34(2)	34(2)	27(1)	-2(2)	2(1)	1(1)
C(1)	20(2)	24(2)	21(1)	1(2)	5(1)	1(1)
C(2)	24(2)	22(2)	21(1)	4(2)	1(1)	2(1)
C(2')	35(3)	22(2)	27(2)	-4(2)	7(1)	-1(1)
C(3)	22(2)	29(2)	21(1)	3(2)	4(1)	4(1)
C(4)	29(3)	28(2)	23(2)	3(2)	4(1)	-3(1)
C(5)	31(3)	26(2)	21(2)	2(2)	0(1)	1(1)
C(6)	23(3)	31(2)	24(2)	-6(2)	2(1)	2(1)
C(7)	33(3)	30(2)	20(1)	-2(2)	4(1)	-1(1)
C(8)	50(3)	50(2)	30(2)	-2(2)	-1(2)	-12(2)
C(9)	24(3)	47(2)	29(2)	-3(2)	-1(1)	0(1)
C(12)	29(3)	33(2)	30(2)	5(2)	11(1)	-2(1)
C(13)	61(3)	37(2)	30(2)	-2(2)	16(2)	-5(1)
C(15)	65(4)	45(2)	22(2)	-5(2)	9(2)	8(1)
C(16)	38(3)	30(2)	24(2)	0(2)	5(1)	4(1)
C(21)	31(3)	22(2)	20(1)	-3(2)	1(1)	2(1)
C(22)	33(3)	24(2)	20(2)	-6(2)	-1(1)	-4(1)
C(22')	48(3)	27(2)	37(2)	-2(2)	-5(2)	8(1)
C(23)	38(3)	27(2)	30(2)	8(2)	5(1)	1(1)
C(24)	31(3)	38(2)	30(2)	-1(2)	5(1)	1(1)

C(25)	29(3)	28(2)	34(2)	-1(2)	8(1)	4(1)
C(26)	30(3)	35(2)	23(2)	0(2)	2(1)	10(1)
C(27)	42(3)	46(2)	31(2)	3(2)	12(2)	6(1)
C(28)	73(4)	56(3)	32(2)	18(2)	14(2)	-2(2)
C(29)	51(4)	72(3)	58(2)	8(3)	25(2)	20(2)
C(32)	31(3)	30(2)	24(2)	6(2)	-3(1)	0(1)
C(33)	33(3)	42(2)	33(2)	-1(2)	5(1)	-5(1)
C(35)	34(3)	44(2)	36(2)	-11(2)	4(1)	-3(2)
C(36)	25(3)	30(2)	29(2)	-9(2)	-1(1)	-3(1)
C(41)	25(2)	17(2)	19(1)	4(1)	0(1)	2(1)
C(42)	26(3)	17(2)	21(1)	-3(2)	7(1)	-3(1)
C(42')	37(3)	24(2)	25(2)	5(2)	3(1)	1(1)
C(43)	25(2)	27(2)	21(1)	-3(2)	4(1)	-4(1)
C(44)	29(3)	24(2)	20(1)	0(2)	0(1)	0(1)
C(45)	31(3)	21(2)	26(2)	6(2)	4(1)	-2(1)
C(46)	28(3)	28(2)	22(2)	4(2)	-1(1)	-3(1)
C(47)	27(3)	28(2)	24(2)	6(2)	3(1)	3(1)
C(48)	34(3)	40(2)	34(2)	8(2)	1(1)	4(1)
C(49)	34(3)	34(2)	33(2)	-2(2)	7(1)	-4(1)
C(52)	27(3)	27(2)	27(2)	-1(2)	5(1)	2(1)
C(53)	36(3)	32(2)	36(2)	1(2)	0(2)	0(1)
C(55)	38(3)	38(2)	31(2)	4(2)	3(1)	11(1)
C(56)	28(3)	29(2)	26(2)	3(2)	6(1)	6(1)
C(61)	35(3)	33(2)	25(2)	4(2)	1(1)	4(1)
C(62)	37(3)	30(2)	25(2)	-2(2)	0(1)	-4(1)
C(62')	57(3)	44(2)	27(2)	6(2)	-5(2)	2(1)
C(63)	40(3)	59(3)	43(2)	-7(2)	3(2)	-14(2)
C(64)	55(4)	39(2)	48(2)	-5(2)	13(2)	-5(2)
C(65)	53(3)	51(2)	29(2)	-6(2)	7(2)	1(2)
C(66)	42(3)	47(2)	29(2)	-2(2)	3(2)	-7(1)
C(67)	50(4)	49(2)	54(2)	1(2)	11(2)	-2(2)
C(68)	59(4)	63(3)	79(3)	11(3)	3(2)	-3(2)
C(69)	81(5)	69(3)	79(3)	-10(3)	39(3)	-9(2)
C(72)	46(3)	62(3)	32(2)	1(2)	0(2)	-2(2)
C(73)	51(4)	91(4)	46(2)	-5(3)	8(2)	-7(2)
C(75)	67(4)	50(2)	38(2)	-13(2)	13(2)	-7(2)
C(76)	52(3)	40(2)	39(2)	-12(2)	7(2)	1(1)

TABLE IV. Hydrogen Fixed Atom Coordinates (Biso=B(attached) +1.0)

H(1)	1680	-929	1976	H(41)	4379	2258	996
H(2)	3482	1747	1722	H(42)	4166	5466	1754
H(2')	1438	4989	1892	H(42')	4521	8161	902
H(2")	2512	5161	1828	H(42')	4300	8425	1353
H(2"')	2244	4246	2240	H(42")	3546	7357	1023
H(3)	2260	2779	1170	H(43)	5797	6191	1648
H(3')	1220	3201	1228	H(43')	6010	6511	1211
H(4)	1964	-860	1017	H(44)	6245	2554	1651
H(5)	746	-2666	1314	H(45)	6057	604	1031
H(6)	99	1352	1591	H(46)	5674	4563	598
H(6')	-4	-928	1804	H(46')	5295	2259	443
H(8)	-216	-2699	481	H(48)	8086	549	1149
H(8')	874	-3180	606	H(48')	7459	200	1502
H(8")	550	-1475	265	H(48")	8292	1894	1552
H(9)	-824	1057	633	H(49)	7971	4253	782

H(9')	36	2355	500	H(49')	7997	5616	1185
H(9")	-201	2535	949	H(49")	7117	5776	843
H(12)	-188	1567	2359	H(52)	3063	1051	622
H(12')	393	3629	2275	H(52')	3593	1249	237
H(13)	994	3853	2973	H(53)	1942	1122	30
H(13')	-112	3922	2924	H(53')	1794	3115	303
H(15)	1189	-1527	3265	H(55)	2410	6575	120
H(15')	1798	460	3182	H(55')	2905	6770	-270
H(16)	1701	-1898	2619	H(56)	4178	4620	41
H(16')	584	-1683	2565	H(56')	4071	6702	303
H(21)	5319	-4506	2548	H(61)	9098	655	4446
H(22)	3776	-1238	2080	H(62)	9438	441	3625
H(22')	5538	1376	2669	H(62')	7766	4267	3715
H(22')	4674	1669	2322	H(62')	8697	3780	3524
H(22")	5606	527	2225	H(62")	7731	2675	3346
H(23)	3531	-339	2734	H(63)	7425	-1367	3874
H(23')	4380	-140	3072	H(63')	6889	577	3780
H(24)	3256	-3917	2904	H(64)	7030	-1294	4516
H(25)	4551	-6111	3175	H(65)	7722	1220	4988
H(26)	5738	-2409	3306	H(66)	8003	4429	4424
H(26')	6087	-4781	3228	H(66')	8712	3809	4812
H(28)	4640	-2472	4065	H(68)	5959	4924	4443
H(28')	3808	-983	3871	H(68')	5529	3198	4123
H(28")	4794	-933	3701	H(68")	6552	4091	4106
H(29)	3630	-5902	3922	H(69)	5733	2320	5053
H(29')	3121	-6278	3475	H(69')	6154	-7	5041
H(29")	2759	-4455	3742	H(69")	5257	626	4733
H(32)	6574	-5703	2265	H(72)	10668	628	4509
H(32')	7194	-5599	2693	H(72')	10651	2753	4769
H(33)	8175	-5582	2176	H(73)	12129	2476	4527
H(33')	7670	-3531	1992	H(73')	11633	2301	4082
H(35)	7884	-153	2382	H(75)	10767	5460	3776
H(35')	8508	-174	2802	H(75')	10784	7536	4032
H(36)	7386	-2340	3068	H(76)	9880	5888	4480
H(36')	6904	-200	2896	H(76')	9342	5858	4034

TABLE V. Interatomic Distances (A)

O(2)-C(2)	1.444 (4)	O(14)-C(15)	1.428 (4)
O(14)-C(13)	1.434 (4)	O(22)-C(22)	1.469 (3)
O(34)-C(33)	1.423 (4)	C(44)-C(47)	1.511 (4)
O(34)-C(35)	1.416 (4)	C(45)-C(46)	1.508 (4)
O(42)-C(42)	1.453 (3)	C(45)-C(47)	1.502 (4)
O(54)-C(53)	1.438 (4)	C(47)-C(48)	1.511 (4)
O(54)-C(55)	1.417 (4)	C(47)-C(49)	1.499 (4)
O(62)-C(62)	1.433 (4)	C(52)-C(53)	1.508 (4)
O(74)-C(73)	1.411 (5)	C(55)-C(56)	1.512 (5)
O(74)-C(75)	1.417 (5)	C(61)-C(62)	1.537 (4)
O(2)-H(2)	0.951 (0)	C(61)-C(66)	1.537 (5)
O(22)-H(22)	0.952 (0)	C(62)-C(62')	1.522 (4)
O(42)-H(42)	0.945 (0)	C(62)-C(63)	1.531 (5)
O(62)-H(62)	0.959 (0)	C(63)-C(64)	1.515 (5)
N(11)-C(1)	1.491 (3)	C(64)-C(65)	1.510 (5)
N(11)-C(12)	1.466 (4)	C(64)-C(67)	1.526 (5)
N(11)-C(16)	1.471 (4)	C(65)-C(66)	1.503 (5)

N(31)-C(21)	1.470 (4)	C(65)-C(67)	1.482 (5)
N(31)-C(32)	1.469 (4)	C(67)-C(68)	1.491 (6)
N(31)-C(36)	1.472 (4)	C(67)-C(69)	1.523 (5)
N(51)-C(41)	1.480 (4)	C(72)-C(73)	1.515 (6)
N(51)-C(52)	1.456 (4)	C(75)-C(76)	1.469 (5)
N(51)-C(56)	1.472 (3)	C(1)-H(1)	0.950 (0)
N(71)-C(61)	1.461 (4)	C(2')-H(2')	0.951 (0)
N(71)-C(72)	1.454 (4)	C(2')-H(2")	0.949 (0)
N(71)-C(76)	1.453 (4)	C(2')-H(2"')	0.949 (0)
C(1)-C(2)	1.541 (4)	C(3)-H(3)	0.951 (0)
C(1)-C(6)	1.539 (4)	C(3)-H(3')	0.952 (0)
C(2)-C(2')	1.530 (4)	C(4)-H(4)	0.948 (0)
C(2)-C(3)	1.549 (4)	C(5)-H(5)	0.952 (0)
C(3)-C(4)	1.500 (4)	C(6)-H(6)	0.952 (0)
C(4)-C(5)	1.523 (4)	C(6)-H(6')	0.950 (0)
C(4)-C(7)	1.515 (4)	C(8)-H(8)	0.953 (0)
C(5)-C(6)	1.511 (4)	C(8)-H(8')	0.952 (0)
C(5)-C(7)	1.515 (4)	C(8)-H(8")	0.947 (0)
C(7)-C(8)	1.518 (4)	C(9)-H(9)	0.951 (0)
C(7)-C(9)	1.496 (5)	C(9)-H(9')	0.949 (0)
C(12)-C(13)	1.510 (4)	C(9)-H(9")	0.951 (0)
C(15)-C(16)	1.511 (4)	C(12)-H(12)	0.951 (0)
C(21)-C(22)	1.564 (4)	C(12)-H(12')	0.949 (0)
C(21)-C(26)	1.542 (4)	C(13)-H(13)	0.947 (0)
C(22)-C(22')	1.507 (4)	C(13)-H(13')	0.952 (0)
C(22)-C(23)	1.528 (4)	C(15)-H(15)	0.948 (0)
C(23)-C(24)	1.508 (4)	C(15)-H(15')	0.952 (0)
C(24)-C(25)	1.512 (5)	C(16)-H(16)	0.951 (0)
C(24)-C(27)	1.520 (4)	C(16)-H(16')	0.951 (0)
C(25)-C(26)	1.502 (5)	C(21)-H(21)	0.951 (0)
C(25)-C(27)	1.513 (5)	C(22')-H(22')	0.949 (0)
C(27)-C(28)	1.510 (5)	C(22')-H(22')	0.949 (0)
C(27)-C(29)	1.507 (5)	C(22')-H(22")	0.951 (0)
C(32)-C(33)	1.489 (5)	C(23)-H(23)	0.951 (0)
C(35)-C(36)	1.502 (5)	C(23)-H(23')	0.949 (0)
C(41)-C(42)	1.561 (4)	C(24)-H(24)	0.950 (0)
C(41)-C(46)	1.528 (4)	C(25)-H(25)	0.952 (0)
C(42)-C(42')	1.519 (4)	C(26)-H(26)	0.948 (0)
C(42)-C(43)	1.520 (4)	C(26)-H(26')	0.953 (0)
C(43)-C(44)	1.502 (4)	C(28)-H(28)	0.952 (0)
C(44)-C(45)	1.519 (4)	C(28)-H(28')	0.948 (0)
C(28)-H(28")	0.949 (0)	C(53)-H(53)	0.951 (0)
C(29)-H(29)	0.951 (0)	C(53)-H(53')	0.951 (0)
C(29)-H(29')	0.947 (0)	C(55)-H(55)	0.950 (0)
C(29)-H(29")	0.951 (0)	C(55)-H(55')	0.949 (0)
C(32)-H(32)	0.952 (0)	C(56)-H(56)	0.951 (0)
C(32)-H(32')	0.951 (0)	C(56)-H(56')	0.950 (0)
C(33)-H(33)	0.955 (0)	C(61)-H(61)	0.950 (0)
C(33)-H(33')	0.949 (0)	C(62')-H(62')	0.948 (0)
C(35)-H(35)	0.950 (0)	C(62')-H(62')	0.953 (0)
C(35)-H(35')	0.950 (0)	C(62')-H(62")	0.949 (0)
C(36)-H(36)	0.951 (0)	C(63)-H(63)	0.949 (0)
C(36)-H(36')	0.950 (0)	C(63)-H(63')	0.951 (0)
C(41)-H(41)	0.951 (0)	C(64)-H(64)	0.949 (0)
C(42')-H(42')	0.948 (0)	C(65)-H(65)	0.951 (0)
C(42')-H(42')	0.948 (0)	C(66)-H(66)	0.949 (0)

C(42’)-H(42")	0.952 (0)	C(66)-H(66’)	0.950 (0)
C(43)-H(43)	0.949 (0)	C(68)-H(68)	0.952 (0)
C(43)-H(43’)	0.949 (0)	C(68)-H(68’)	0.951 (0)
C(44)-H(44)	0.950 (0)	C(68)-H(68")	0.950 (0)
C(45)-H(45)	0.950 (0)	C(69)-H(69)	0.952 (0)
C(46)-H(46)	0.951 (0)	C(69)-H(69’)	0.947 (0)
C(46)-H(46’)	0.951 (0)	C(69)-H(69")	0.951 (0)
C(48)-H(48)	0.949 (0)	C(72)-H(72)	0.950 (0)
C(48)-H(48’)	0.949 (0)	C(72)-H(72’)	0.951 (0)
C(48)-H(48")	0.949 (0)	C(73)-H(73)	0.949 (0)
C(49)-H(49)	0.950 (0)	C(73)-H(73’)	0.953 (0)
C(49)-H(49’)	0.948 (0)	C(75)-H(75)	0.948 (0)
C(49)-H(49")	0.952 (0)	C(75)-H(75’)	0.952 (0)
C(52)-H(52)	0.950 (0)	C(76)-H(76)	0.949 (0)
C(52)-H(52’)	0.952 (0)	C(76)-H(76’)	0.950 (0)

TABLE VI. Intramolecular Angles (Deg)

C(13)-O(14)-C(15)	109.8 (2)	O(74)-C(75)-H(75’)	110 (0)
C(33)-O(34)-C(35)	109.9 (3)	N(11)-C(1)-C(2)	113.0 (2)
C(53)-O(54)-C(55)	109.8 (2)	N(11)-C(1)-C(6)	114.9 (3)
C(73)-O(74)-C(75)	109.8 (3)	N(11)-C(12)-C(13)	109.5 (3)
C(2)-O(2)-H(2)	119 (0)	N(11)-C(16)-C(15)	109.1 (3)
C(22)-O(22)-H(22)	103 (0)	N(31)-C(21)-C(22)	113.7 (2)
C(42)-O(42)-H(42)	106 (0)	N(31)-C(21)-C(26)	115.4 (3)
C(62)-O(62)-H(62)	107 (0)	N(31)-C(32)-C(33)	110.2 (3)
C(1)-N(11)-C(16)	111.7 (2)	N(31)-C(36)-C(35)	110.0 (2)
C(1)-N(11)-C(12)	115.9 (2)	N(51)-C(41)-C(42)	114.1 (2)
C(12)-N(11)-C(16)	107.5 (2)	N(51)-C(41)-C(46)	115.8 (2)
C(21)-N(31)-C(32)	113.4 (2)	N(51)-C(52)-C(53)	110.3 (3)
C(21)-N(31)-C(36)	115.7 (2)	N(51)-C(56)-C(55)	109.0 (3)
C(32)-N(31)-C(36)	106.5 (3)	N(71)-C(61)-C(62)	110.0 (2)
C(41)-N(51)-C(56)	114.7 (3)	N(71)-C(61)-C(66)	118.0 (3)
C(41)-N(51)-C(52)	112.2 (2)	N(71)-C(72)-C(73)	109.2 (3)
C(52)-N(51)-C(56)	107.0 (2)	N(71)-C(76)-C(75)	109.2 (3)
C(61)-N(71)-C(72)	113.6 (3)	N(11)-C(1)-H(1)	105 (0)
C(61)-N(71)-C(76)	116.9 (3)	N(11)-C(12)-H(12’)	109 (0)
C(72)-N(71)-C(76)	107.8 (3)	N(11)-C(12)-H(12)	109 (0)
O(2)-C(2)-C(3)	107.8 (2)	N(11)-C(16)-H(16)	110 (0)
O(2)-C(2)-C(1)	106.0 (2)	N(11)-C(16)-H(16’)	109 (0)
O(2)-C(2)-C(2’)	108.4 (2)	N(31)-C(21)-H(21)	106 (0)
O(14)-C(13)-C(12)	111.0 (3)	N(31)-C(32)-H(32)	109 (0)
O(14)-C(15)-C(16)	111.8 (3)	N(31)-C(32)-H(32’)	110 (0)
O(22)-C(22)-C(21)	104.4 (2)	N(31)-C(36)-H(36)	109 (0)
O(22)-C(22)-C(23)	107.6 (3)	N(31)-C(36)-H(36’)	110 (0)
O(22)-C(22)-C(22’)	108.3 (2)	N(51)-C(41)-H(41)	105 (0)
O(34)-C(33)-C(32)	112.0 (2)	N(51)-C(52)-H(52’)	110 (0)
O(34)-C(35)-C(36)	112.3 (3)	N(51)-C(52)-H(52)	109 (0)
O(42)-C(42)-C(43)	108.6 (2)	N(51)-C(56)-H(56’)	110 (0)
O(42)-C(42)-C(42’)	108.2 (2)	N(51)-C(56)-H(56)	110 (0)
O(42)-C(42)-C(41)	105.1 (2)	N(71)-C(61)-H(61)	106 (0)
O(54)-C(53)-C(52)	110.8 (3)	N(71)-C(72)-H(72’)	109 (0)
O(54)-C(55)-C(56)	111.0 (3)	N(71)-C(72)-H(72)	110 (0)
O(62)-C(62)-C(62’)	107.2 (2)	N(71)-C(76)-H(76’)	109 (0)
O(62)-C(62)-C(61)	108.9 (3)	N(71)-C(76)-H(76)	110 (0)

O(62)-C(62)-C(63)	105.2 (3)	C(2)-C(1)-C(6)	112.3 (2)
O(74)-C(73)-C(72)	112.1 (4)	C(1)-C(2)-C(3)	111.2 (2)
O(74)-C(75)-C(76)	112.0 (3)	C(1)-C(2)-C(2')	114.5 (2)
O(14)-C(13)-H(13)	110 (0)	C(2')-C(2)-C(3)	108.8 (2)
O(14)-C(13)-H(13')	109 (0)	C(2)-C(3)-C(4)	113.0 (2)
O(14)-C(15)-H(15')	110 (0)	C(3)-C(4)-C(7)	120.5 (3)
O(14)-C(15)-H(15)	110 (0)	C(3)-C(4)-C(5)	112.7 (3)
O(34)-C(33)-H(33)	110 (0)	C(5)-C(4)-C(7)	59.8 (2)
O(34)-C(33)-H(33')	110 (0)	C(4)-C(5)-C(7)	59.8 (2)
O(34)-C(35)-H(35)	110 (0)	C(4)-C(5)-C(6)	114.0 (3)
O(34)-C(35)-H(35')	110 (0)	C(6)-C(5)-C(7)	126.5 (3)
O(54)-C(53)-H(53)	109 (0)	C(1)-C(6)-C(5)	107.1 (3)
O(54)-C(53)-H(53')	110 (0)	C(4)-C(7)-C(9)	121.9 (3)
O(54)-C(55)-H(55')	110 (0)	C(4)-C(7)-C(8)	115.0 (3)
O(54)-C(55)-H(55)	110 (0)	C(4)-C(7)-C(5)	60.3 (2)
O(74)-C(73)-H(73')	110 (0)	C(5)-C(7)-C(9)	123.0 (3)
O(74)-C(73)-H(73)	110 (0)	C(5)-C(7)-C(8)	114.4 (3)
O(74)-C(75)-H(75)	110 (0)	C(8)-C(7)-C(9)	112.8 (3)
C(22)-C(21)-C(26)	111.3 (2)	C(2)-C(2')-H(2")	109 (0)
C(21)-C(22)-C(22')	114.6 (3)	C(2)-C(2')-H(2"')	110 (0)
C(21)-C(22)-C(23)	112.1 (2)	C(2)-C(2')-H(2')	110 (0)
C(22')-C(22)-C(23)	109.5 (3)	C(2)-C(3)-H(3)	109 (0)
C(22)-C(23)-C(24)	113.2 (3)	C(2)-C(3)-H(3')	110 (0)
C(23)-C(24)-C(25)	113.4 (3)	C(4)-C(3)-H(3)	109 (0)
C(23)-C(24)-C(27)	122.4 (3)	C(4)-C(3)-H(3')	110 (0)
C(25)-C(24)-C(27)	59.9 (2)	C(3)-C(4)-H(4)	117 (0)
C(24)-C(25)-C(27)	60.3 (2)	C(5)-C(4)-H(4)	117 (0)
C(24)-C(25)-C(26)	114.1 (3)	C(7)-C(4)-H(4)	117 (0)
C(26)-C(25)-C(27)	125.9 (3)	C(4)-C(5)-H(5)	115 (0)
C(21)-C(26)-C(25)	108.2 (3)	C(6)-C(5)-H(5)	114 (0)
C(24)-C(27)-C(28)	121.0 (3)	C(7)-C(5)-H(5)	115 (0)
C(24)-C(27)-C(29)	115.7 (3)	C(1)-C(6)-H(6')	110 (0)
C(24)-C(27)-C(25)	59.8 (2)	C(1)-C(6)-H(6)	109 (0)
C(25)-C(27)-C(28)	121.2 (3)	C(5)-C(6)-H(6')	110 (0)
C(25)-C(27)-C(29)	115.3 (3)	C(5)-C(6)-H(6)	109 (0)
C(28)-C(27)-C(29)	113.6 (3)	C(7)-C(8)-H(8')	109 (0)
C(42)-C(41)-C(46)	111.4 (3)	C(7)-C(8)-H(8)	110 (0)
C(41)-C(42)-C(43)	110.7 (2)	C(7)-C(8)-H(8")	110 (0)
C(41)-C(42)-C(42')	114.0 (2)	C(7)-C(9)-H(9')	110 (0)
C(42')-C(42)-C(43)	110.0 (2)	C(7)-C(9)-H(9)	110 (0)
C(42)-C(43)-C(44)	113.6 (2)	C(7)-C(9)-H(9")	110 (0)
C(43)-C(44)-C(45)	113.4 (2)	C(13)-C(12)-H(12)	110 (0)
C(43)-C(44)-C(47)	122.7 (3)	C(13)-C(12)-H(12')	110 (0)
C(45)-C(44)-C(47)	59.4 (2)	C(12)-C(13)-H(13')	109 (0)
C(44)-C(45)-C(47)	60.0 (2)	C(12)-C(13)-H(13)	110 (0)
C(44)-C(45)-C(46)	112.4 (3)	C(16)-C(15)-H(15')	108 (0)
C(46)-C(45)-C(47)	126.6 (3)	C(16)-C(15)-H(15)	109 (0)
C(41)-C(46)-C(45)	107.6 (2)	C(15)-C(16)-H(16)	111 (0)
C(44)-C(47)-C(45)	60.6 (2)	C(15)-C(16)-H(16')	109 (0)
C(44)-C(47)-C(48)	114.6 (2)	C(22)-C(21)-H(21)	105 (0)
C(44)-C(47)-C(49)	121.4 (3)	C(26)-C(21)-H(21)	105 (0)
C(45)-C(47)-C(48)	113.4 (3)	C(22)-C(22')-H(22')	109 (0)
C(45)-C(47)-C(49)	122.7 (3)	C(22)-C(22')-H(22")	110 (0)
C(48)-C(47)-C(49)	114.0 (3)	C(22)-C(22')-H(22')	110 (0)
C(62)-C(61)-C(66)	111.4 (3)	C(22)-C(23)-H(23')	109 (0)
C(61)-C(62)-C(62')	112.9 (3)	C(22)-C(23)-H(23)	110 (0)

C(61)-C(62)-C(63)	110.6 (2)	C(24)-C(23)-H(23)	109 (0)
C(62')-C(62)-C(63)	111.7 (3)	C(24)-C(23)-H(23')	110 (0)
C(62)-C(63)-C(64)	119.8 (3)	C(23)-C(24)-H(24)	116 (0)
C(63)-C(64)-C(65)	119.3 (3)	C(25)-C(24)-H(24)	116 (0)
C(63)-C(64)-C(67)	124.6 (3)	C(27)-C(24)-H(24)	116 (0)
C(65)-C(64)-C(67)	58.4 (2)	C(24)-C(25)-H(25)	115 (0)
C(64)-C(65)-C(67)	61.3 (3)	C(26)-C(25)-H(25)	115 (0)
C(64)-C(65)-C(66)	116.4 (3)	C(27)-C(25)-H(25)	114 (0)
C(66)-C(65)-C(67)	125.4 (3)	C(21)-C(26)-H(26)	110 (0)
C(61)-C(66)-C(65)	110.0 (3)	C(21)-C(26)-H(26')	109 (0)
C(64)-C(67)-C(65)	60.2 (3)	C(25)-C(26)-H(26)	110 (0)
C(64)-C(67)-C(69)	115.5 (3)	C(25)-C(26)-H(26')	109 (0)
C(64)-C(67)-C(68)	119.6 (3)	C(27)-C(28)-H(28')	109 (0)
C(65)-C(67)-C(69)	115.6 (4)	C(27)-C(28)-H(28)	109 (0)
C(65)-C(67)-C(68)	120.8 (4)	C(27)-C(28)-H(28'')	110 (0)
C(68)-C(67)-C(69)	114.5 (4)	C(27)-C(29)-H(29'')	109 (0)
C(2)-C(1)-H(1)	105 (0)	C(27)-C(29)-H(29')	109 (0)
C(6)-C(1)-H(1)	105 (0)	C(27)-C(29)-H(29)	110 (0)
C(33)-C(32)-H(32)	110 (0)	C(73)-C(72)-H(72')	109 (0)
C(33)-C(32)-H(32')	109 (0)	C(72)-C(73)-H(73')	109 (0)
C(32)-C(33)-H(33')	109 (0)	C(72)-C(73)-H(73)	109 (0)
C(32)-C(33)-H(33)	110 (0)	C(76)-C(75)-H(75')	109 (0)
C(36)-C(35)-H(35')	109 (0)	C(76)-C(75)-H(75)	110 (0)
C(36)-C(35)-H(35)	109 (0)	C(75)-C(76)-H(76')	109 (0)
C(35)-C(36)-H(36')	110 (0)	C(75)-C(76)-H(76)	110 (0)
C(35)-C(36)-H(36)	109 (0)	H(2')-C(2')-H(2'')	110 (0)
C(42)-C(41)-H(41)	104 (0)	H(2')-C(2')-H(2''')	109 (0)
C(46)-C(41)-H(41)	105 (0)	H(2''')-C(2')-H(2'')	109 (0)
C(42)-C(42')-H(42')	110 (0)	H(3)-C(3)-H(3')	106 (0)
C(42)-C(42')-H(42')	110 (0)	H(6)-C(6)-H(6')	112 (0)
C(42)-C(42')-H(42'')	109 (0)	H(8)-C(8)-H(8')	109 (0)
C(42)-C(43)-H(43)	109 (0)	H(8)-C(8)-H(8'')	110 (0)
C(42)-C(43)-H(43')	109 (0)	H(8')-C(8)-H(8'')	109 (0)
C(44)-C(43)-H(43')	110 (0)	H(9)-C(9)-H(9')	109 (0)
C(44)-C(43)-H(43)	109 (0)	H(9)-C(9)-H(9'')	109 (0)
C(43)-C(44)-H(44)	117 (0)	H(9')-C(9)-H(9'')	109 (0)
C(45)-C(44)-H(44)	116 (0)	H(12)-C(12)-H(12')	109 (0)
C(47)-C(44)-H(44)	116 (0)	H(13)-C(13)-H(13')	108 (0)
C(44)-C(45)-H(45)	115 (0)	H(15)-C(15)-H(15')	107 (0)
C(46)-C(45)-H(45)	115 (0)	H(16)-C(16)-H(16')	110 (0)
C(47)-C(45)-H(45)	115 (0)	H(22')-C(22')-H(22'')	109 (0)
C(41)-C(46)-H(46')	110 (0)	H(22')-C(22')-H(22')	110 (0)
C(41)-C(46)-H(46)	109 (0)	H(22')-C(22')-H(22'')	109 (0)
C(45)-C(46)-H(46)	110 (0)	H(23)-C(23)-H(23')	106 (0)
C(45)-C(46)-H(46')	110 (0)	H(26)-C(26)-H(26')	111 (0)
C(47)-C(48)-H(48)	109 (0)	H(28)-C(28)-H(28'')	110 (0)
C(47)-C(48)-H(48'')	109 (0)	H(28)-C(28)-H(28')	109 (0)
C(47)-C(48)-H(48')	110 (0)	H(28')-C(28)-H(28'')	110 (0)
C(47)-C(49)-H(49')	110 (0)	H(29)-C(29)-H(29'')	110 (0)
C(47)-C(49)-H(49'')	109 (0)	H(29)-C(29)-H(29')	109 (0)
C(47)-C(49)-H(49)	109 (0)	H(29')-C(29)-H(29'')	109 (0)
C(53)-C(52)-H(52)	109 (0)	H(32)-C(32)-H(32')	108 (0)
C(53)-C(52)-H(52')	110 (0)	H(33)-C(33)-H(33')	106 (0)
C(52)-C(53)-H(53')	110 (0)	H(35)-C(35)-H(35')	106 (0)
C(52)-C(53)-H(53)	109 (0)	H(36)-C(36)-H(36')	109 (0)
C(56)-C(55)-H(55)	109 (0)	H(42')-C(42')-H(42'')	109 (0)

C(56)-C(55)-H(55')	109 (0)	H(42')-C(42')-H(42')	110 (0)
C(55)-C(56)-H(56)	109 (0)	H(42')-C(42')-H(42")	109 (0)
C(55)-C(56)-H(56')	109 (0)	H(43)-C(43)-H(43')	105 (0)
C(62)-C(61)-H(61)	105 (0)	H(46)-C(46)-H(46')	111 (0)
C(66)-C(61)-H(61)	105 (0)	H(48)-C(48)-H(48")	109 (0)
C(62)-C(62')-H(62')	110 (0)	H(48)-C(48)-H(48')	110 (0)
C(62)-C(62')-H(62')	110 (0)	H(48')-C(48)-H(48")	110 (0)
C(62)-C(62')-H(62")	110 (0)	H(49)-C(49)-H(49')	110 (0)
C(62)-C(63)-H(63)	110 (0)	H(49)-C(49)-H(49")	109 (0)
C(62)-C(63)-H(63')	109 (0)	H(49')-C(49)-H(49")	109 (0)
C(64)-C(63)-H(63')	109 (0)	H(52)-C(52)-H(52')	109 (0)
C(64)-C(63)-H(63)	110 (0)	H(53)-C(53)-H(53')	108 (0)
C(63)-C(64)-H(64)	114 (0)	H(55)-C(55)-H(55')	108 (0)
C(65)-C(64)-H(64)	115 (0)	H(56)-C(56)-H(56')	110 (0)
C(67)-C(64)-H(64)	114 (0)	H(62')-C(62')-H(62")	109 (0)
C(64)-C(65)-H(65)	114 (0)	H(62')-C(62')-H(62')	109 (0)
C(66)-C(65)-H(65)	114 (0)	H(62')-C(62')-H(62")	109 (0)
C(67)-C(65)-H(65)	115 (0)	H(63)-C(63)-H(63')	97 (0)
C(61)-C(66)-H(66')	110 (0)	H(66)-C(66)-H(66')	109 (0)
C(61)-C(66)-H(66)	109 (0)	H(68)-C(68)-H(68")	109 (0)
C(65)-C(66)-H(66)	109 (0)	H(68)-C(68)-H(68')	109 (0)
C(65)-C(66)-H(66')	110 (0)	H(68')-C(68)-H(68")	108 (0)
C(67)-C(68)-H(68')	110 (0)	H(69)-C(69)-H(69')	109 (0)
C(67)-C(68)-H(68)	111 (0)	H(69)-C(69)-H(69")	110 (0)
C(67)-C(68)-H(68")	110 (0)	H(69')-C(69)-H(69")	109 (0)
C(67)-C(69)-H(69')	110 (0)	H(72)-C(72)-H(72')	110 (0)
C(67)-C(69)-H(69")	110 (0)	H(73)-C(73)-H(73')	107 (0)
C(67)-C(69)-H(69)	110 (0)	H(75)-C(75)-H(75')	106 (0)
C(73)-C(72)-H(72)	110 (0)	H(76)-C(76)-H(76')	109 (0)

TABLE VII. Intramolecular Non-Bonding Distances (A)

O(2)...C(5)	3.730 (4)
O(22)...C(25)	3.675 (3)
O(42)...C(45)	3.734 (4)
O(62)...C(72)	3.711 (4)
C(2')...C(12)	3.235 (5)
C(22')...C(36)	3.233 (5)
C(42')...C(56)	3.220 (4)
C(62')...C(76)	3.258 (5)

TABLE VIII. Intermolecular Distances (A)

O(2)...O(22)	2.857 (3)
O(2)...O(42)	2.860 (3)
O(14)...O(62)a	3.087 (3)
O(22)...O(42)b	2.834 (3)
O(42)...C(2')	3.387 (4)
O(62)...C(76)b	3.385 (4)
O(74)...C(29)c	3.350 (5)
O(74)...C(65)d	3.380 (4)
O(2)...H(22)	1.911 (0)
O(22)...H(42)b	1.891 (0)
O(42)...H(2)	1.987 (0)

Symmetry Operation Codes

a	-1+X,Y,Z	c	1+X,1+Y,Z
b	X,-1+Y,Z	d	2-X,1/2+Y,1-Z